



chain nodes :

7 9 16 29 34 35 37 74

ring nodes :

1 2 3 4 5 6 10 11 12 13 14 15 17 18 19 20 21 22 23 24 25 26 27 28 38
39 40 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66

67 68

chain bonds :

1-34 4-35 7-9 7-14 16-21 27-29 35-37 37-74

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-38 6-40 10-11 10-15 11-12 12-13 13-14 14-15 17-18
17-22 18-19 19-20 20-21 21-22 23-24 23-28 24-25 25-26 26-27 27-28 38-39 39-40
45-46 45-50 46-47 47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55 55-56 57-58
57-62 58-59 59-60 60-61 61-62 63-64 63-68 64-65 65-66 66-67 67-68

exact/norm bonds :

1-34 4-35 5-38 6-40 7-9 7-14 10-11 10-15 11-12 12-13 13-14 14-15 16-21 17-18
17-22 18-19 19-20 20-21 21-22 23-24 23-28 24-25 25-26 26-27 27-28 27-29 35-37
37-74 38-39 39-40

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 45-46 45-50 46-47 47-48 48-49 49-50 51-52 51-56 52-53
53-54 54-55 55-56 57-58 57-62 58-59 59-60 60-61 61-62 63-64 63-68 64-65 65-66
66-67 67-68

G2:O,S,N

G3:[*1],[*2],[*3]

G4:C,S,N

G5:C,N

G6:Cb,[*4],[*5],[*6],[*7]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:Atom 11:Atom 12:Atom
13:Atom

14:Atom 15:Atom 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 34:CLASS 35:CLASS 37:CLASS
38:Atom 39:Atom 40:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom
52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom
62:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 74:CLASS